

# Vacancy Electromigration in IC Interconnect Lines

## Introduction

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As integrated circuits (ICs) continue to become more powerful and designed to fit into smaller footprints, it is increasingly important to identify and prevent any cause of circuit failure. One such failure mechanism is due to electromigration effects within the circuit's interconnects.

Electromigration refers to the mass transport due to momentum transfer between electrons and metal atoms. Diffusion in solids occurs due to atoms moving into neighboring vacancies. The migration and accumulation of vacancies within the metal can lead to failure, as voids increase the resistance of the line which in turn cause the severing of the circuit.

Electromigration is inherently multiphysics in nature, as it includes the transport of vacancies due to concentration, stress, potential, and temperature gradients. This example shows how to include all these effects. The results are compared with the values in [Ref. 1](#).

## Model Definition

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The model geometry consists of a small metal stripe 50  $\mu\text{m}$  wide and 15  $\mu\text{m}$  high. The left side is connected to ground, a normal current density of 0.01  $\text{A}/\mu\text{m}^2$  is applied on the right side, while the top and bottom boundaries are insulated. The displacement are constrained on all boundaries. No-flux boundary condition is used for the vacancy transport on all boundaries. The temperature is held fixed at 473 K on both left and right boundaries, to validate the results given in [Ref. 1](#).

The vacancy transport is given by the balance equation:

$$\frac{\partial c_v}{\partial t} + \nabla \cdot \mathbf{j}_v = G$$

The vacancy flux  $\mathbf{j}_v$  considers the effect of the vacancy concentration gradient,  $\nabla c_v$ , the drift velocity,  $\mathbf{v}_d$ , the hydrostatic stress gradient,  $\nabla \sigma$ , and the temperature gradient,  $\nabla T$

$$\mathbf{j}_v = -D_v \nabla c_v + c_v \mathbf{v}_d - \frac{f\Omega}{kT} D_v c_v \nabla \sigma_h - \frac{Q}{kT^2} D_v c_v \nabla T$$

here,  $D_v$  is the diffusivity,  $\Omega$  is the atomic volume,  $Q$  is the heat of transport, and  $k$  is Boltzmann constant. The hydrostatic stress is positive in tension, and it is computed from the trace of the stress tensor  $\sigma_h = \text{trace}(\sigma)/3$ .

The drift velocity  $\mathbf{v}_d$  due to the electric field  $\mathbf{E}$  reads

$$\mathbf{v}_d = \frac{D_v}{kT} |z| e \mathbf{E}$$

where  $e$  is the elementary charge and  $z$  is the effective charge number of vacancies.

The electric field in the interconnect is proportional to the electric current density

$$\mathbf{E} = \rho_e \mathbf{j}_e$$

where  $\rho_e$  is the resistivity of the metal, which in this example depends on the temperature.

The *Rosenberg-Ohring recombination* term  $G$  describes the vacancy generation and annihilation, and it depends on the relaxation time  $\tau$  of the deviation in vacancy concentration  $c_v$  with respect to the equilibrium concentration  $c_{v,eq}$

$$G = \frac{c_v - c_{v,eq}}{\tau}$$

Assuming local equilibrium between the vacancy concentration and pressure, the equilibrium concentration is written as

$$c_{v,eq} = c_{v0} \exp\left(\frac{(1-f)\sigma_h \Omega}{kT}\right)$$

where the parameter  $f$  is the average vacancy relaxation ratio, and  $c_{v0}$  is the reference vacancy concentration in the absence of stresses.

A volumetric strain is produced in the lattice by the influx of vacancies:

$$\frac{\partial \epsilon_{vol}}{\partial t} = \Omega (f \nabla \cdot \mathbf{j}_v + (1-f)G)$$

The model parameters are listed in [Table 1](#).

TABLE 1: MODEL PARAMETERS

Parameter	Value
Initial vacancy concentration ( $c_{v0}$ )	6020 $1/\mu\text{m}^3$
Diffusivity ( $D_v$ )	$2.7e^{-10} \text{ m}^2/\text{s}$
Average vacancy relaxation ratio ( $f$ )	0.6
Vacancy relaxation time ( $\tau$ )	$1.8e^{-3} \text{ s}$
Current density ( $\mathbf{j}_e$ )	$0.01 \text{ A}/\mu\text{m}^2$
Effective charge number of vacancies ( $z$ )	4

TABLE I: MODEL PARAMETERS

Parameter	Value
Temperature (T)	473 K
Heat of transport (Q)	0.00094 eV

### Results and Discussion

Figure 1 and Figure 2 show the build-up of hydrostatic stress and vacancy concentration on the anode and cathode versus time.

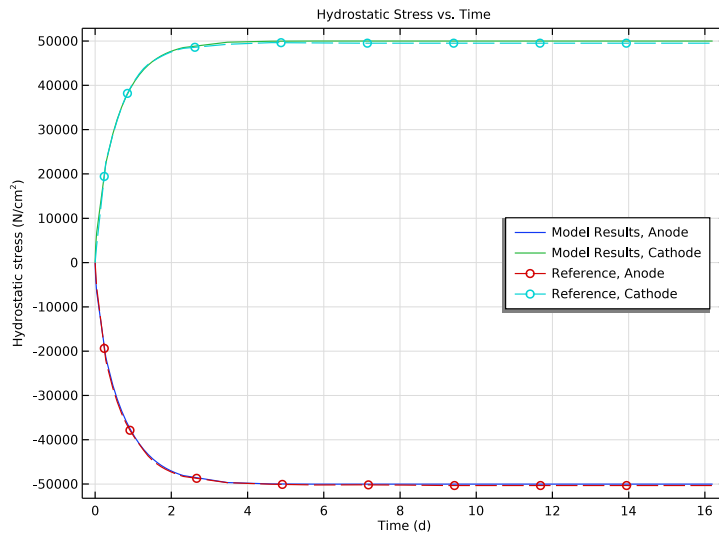


Figure 1: Hydrostatic stress at the center line on the anode and cathode.

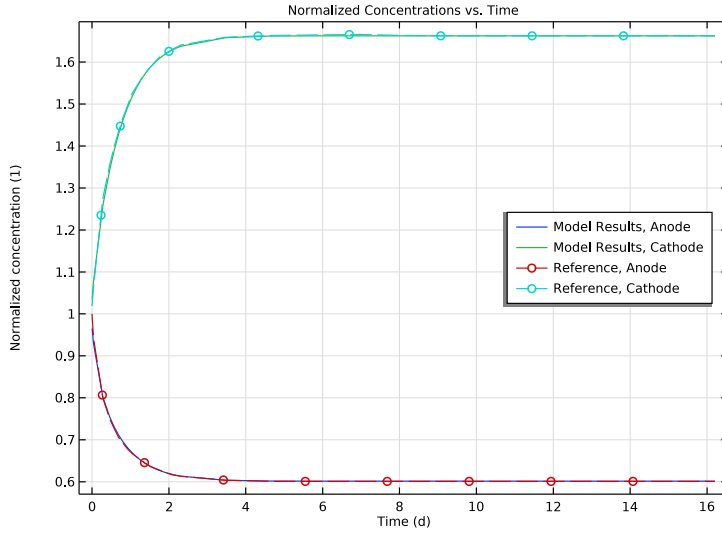


Figure 2: Normalized concentration at the center line on the anode and cathode.

Figure 3 shows the hydrostatic stress on the centerline after 70 s.

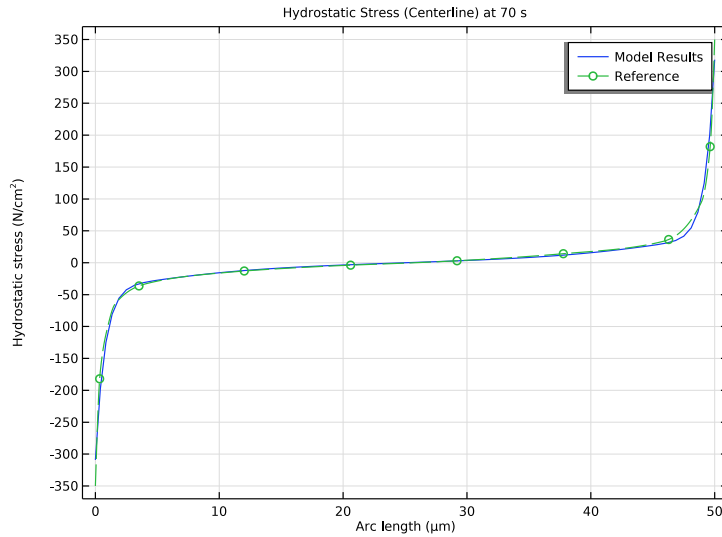
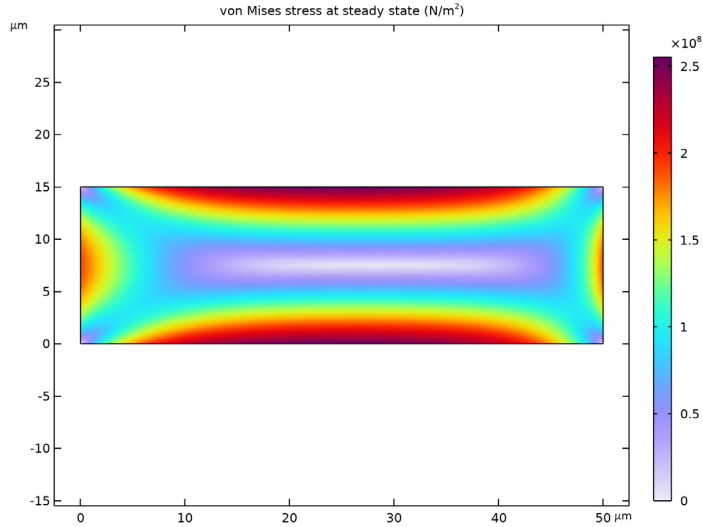


Figure 3: Hydrostatic stress at centerline at 70 s.

The von Mises stress at steady state is shown in [Figure 4](#).



*Figure 4: von Mises stress at steady state.*

### *Notes About the COMSOL Implementation*

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The stress, temperature, and potential contribution to the vacancy flux are included through the **External Flux** feature in the Transport in Solids interface. The vacancy-dependent volumetric deformation is included in the Solid Mechanics interface through the **External Strain** feature.

### *References*

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1. H. Ye, C. Basaran, and D.C. Hopkins, “Numerical simulation of stress evolution during electromigration in IC interconnect lines,” *IEEE Transactions on Components and Packaging Technologies*, vol. 26, no. 3, pp. 673–681, 2003.
2. R.L. Orio, H. Ceric, and S. Selberherr, “Physically based models of electromigration: from Black’s equation to modern TCAD models,” *Microelectron. Reliab.*, vol. 50, no. 6, pp. 775–789, 2010.

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**Application Library path:** Structural\_Mechanics\_Module/Diffusion\_in\_Solids/  
vacancy\_electromigration


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### *Modeling Instructions*




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From the **File** menu, choose **New**.

#### **NEW**

In the **New** window, click  **Model Wizard**.

#### **MODEL WIZARD**

- 1 In the **Model Wizard** window, click  **2D**.
- 2 In the **Select Physics** tree, select **Structural Mechanics > Solid Mechanics (solid)**.
- 3 Click **Add**.
- 4 In the **Select Physics** tree, select **Chemical Species Transport > Transport in Solids (ts)**.
- 5 Click **Add**.
- 6 In the **Select Physics** tree, select **AC/DC > Electric Fields and Currents > Electric Currents (ec)**.
- 7 Click **Add**.
- 8 In the **Select Physics** tree, select **Heat Transfer > Heat Transfer in Solids (ht)**.
- 9 Click **Add**.
- 10 In the **Select Physics** tree, select **Mathematics > ODE and DAE Interfaces > Domain ODEs and DAEs (dode)**.
- 11 Click **Add**.
- 12 Click  **Study**.
- 13 In the **Select Study** tree, select **General Studies > Time Dependent**.
- 14 Click  **Done**.

#### **GLOBAL DEFINITIONS**

##### *Geometric Parameters*

- 1 In the **Model Builder** window, under **Global Definitions** click **Parameters I**.
- 2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 In the table, enter the following settings:

Name	Expression	Value	Description
Height	15[um]	1.5E-5 m	Height
Thick	1[m]	1 m	Out-of-plane thickness
Width	50[um]	5E-5 m	Width

4 In the **Label** text field, type Geometric Parameters.

#### Transport Parameters

1 In the **Home** toolbar, click **Pi Parameters** and choose **Add > Parameters**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 In the table, enter the following settings:

Name	Expression	Value	Description
Cv0	6020[um^-3]	6.02E21 1/m <sup>3</sup>	Initial vacancy concentration
Cv0moles	Cv0/N_A_const	0.0099964 mol/m <sup>3</sup>	Initial vacancy concentration (mol/m <sup>3</sup> )
Dv	2.7e-6[cm^2/s]	2.7E-10 m <sup>2</sup> /s	Diffusivity
taus	1.8e-3[s]	0.0018 s	Vacancy relaxation time
f	.6	0.6	Average vacancy relaxation ratio

4 In the **Label** text field, type Transport Parameters.

#### Electric Currents Parameters

1 In the **Home** toolbar, click **Pi Parameters** and choose **Add > Parameters**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 In the table, enter the following settings:

Name	Expression	Value	Description
Jden	0.01[A/um^2]	1E10 A/m <sup>2</sup>	Current density
Va	1.66e7[pm^3]	1.66E-29 m <sup>3</sup>	Atomic volume
Znum	4	4	Effective charge number
Zref	50[ohm]	50 Ω	Reference impedance



Name	Expression	Value	Description
rho_res	0.03132 [ohm*um]	3.132E-8 Ω·m	Reference resistivity
alpha_res	0.0036367 [1/K]	0.0036367 1/K	Resistivity temperature coefficient

4 In the **Label** text field, type Electric Currents Parameters.

#### Heat Transfer Parameters

1 In the **Home** toolbar, click  **Parameters** and choose **Add > Parameters**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 In the table, enter the following settings:

Name	Expression	Value	Description
Qstar	.00094[eV]	1.506E-22 J	Heat of transport
T0	473[K]	473 K	Initial temperature
Tref	293.15[K]	293.15 K	Reference temperature

4 In the **Label** text field, type Heat Transfer Parameters.

Load the reference data.

#### Hydrostatic Stress at t=70[s]

1 In the **Home** toolbar, click  **Functions** and choose **Global > Interpolation**.

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

3 From the **Data source** list, choose **File**.

4 Click  **Browse**.

5 Browse to the model's Application Libraries folder and double-click the file vacancy\_electromigration\_hydrostatic\_stress.txt.

6 Locate the **Interpolation and Extrapolation** section. From the **Interpolation** list, choose **Piecewise cubic**.

7 Locate the **Data Column Settings** section. In the table, click to select the cell at row number 1 and column number 1.



8 In the **Unit** text field, type um.

9 In the table, click to select the cell at row number 2 and column number 1.



10 In the **Unit** text field, type N/cm<sup>2</sup>.

11 In the **Label** text field, type Hydrostatic Stress at t=70[s].

### *Steady State Hydrostatic Stress*


- 1 In the **Home** toolbar, click  **Functions** and choose **Global > Interpolation**.
- 2 In the **Settings** window for **Interpolation**, locate the **Definition** section.
- 3 From the **Data source** list, choose **File**.
- 4 Click  **Browse**.
- 5 Browse to the model's Application Libraries folder and double-click the file `vacancy_electromigration_hydrostatic_stress_steady.txt`.
- 6 Locate the **Interpolation and Extrapolation** section. From the **Interpolation** list, choose **Piecewise cubic**.
- 7 Locate the **Data Column Settings** section. In the table, click to select the cell at row number 1 and column number 1.
- 8 In the **Unit** text field, type `um`.
- 9 In the table, click to select the cell at row number 2 and column number 1.
- 10 In the **Unit** text field, type `N/cm^2`.
- 11 In the **Label** text field, type `Steady State Hydrostatic Stress`.

### *Stress vs. Time, Anode*



- 1 In the **Home** toolbar, click  **Functions** and choose **Global > Interpolation**.
- 2 In the **Settings** window for **Interpolation**, locate the **Definition** section.
- 3 From the **Data source** list, choose **File**.
- 4 Click  **Browse**.
- 5 Browse to the model's Application Libraries folder and double-click the file `vacancy_electromigration_anode_stress.txt`.
- 6 Locate the **Interpolation and Extrapolation** section. From the **Interpolation** list, choose **Piecewise cubic**.
- 7 Locate the **Data Column Settings** section. In the table, click to select the cell at row number 1 and column number 1.
- 8 In the **Unit** text field, type `s`.
- 9 In the table, click to select the cell at row number 2 and column number 1.
- 10 In the **Unit** text field, type `N/cm^2`.
- 11 In the **Label** text field, type `Stress vs. Time, Anode`.

### *Stress vs. Time, Cathode*



- 1 In the **Home** toolbar, click  **Functions** and choose **Global > Interpolation**.

- 2 In the **Settings** window for **Interpolation**, locate the **Definition** section.
- 3 From the **Data source** list, choose **File**.
- 4 Click  **Browse**.
- 5 Browse to the model's Application Libraries folder and double-click the file `vacancy_electromigration_cathode_stress.txt`.
- 6 Locate the **Interpolation and Extrapolation** section. From the **Interpolation** list, choose **Piecewise cubic**.
- 7 Locate the **Data Column Settings** section. In the table, click to select the cell at row number 1 and column number 1.
- 8 In the **Unit** text field, type `s`.
- 9 In the table, click to select the cell at row number 2 and column number 1.
- 10 In the **Unit** text field, type `N/cm^2`.
- 11 In the **Label** text field, type `Stress vs. Time, Cathode`.

*Concentration vs. Time, Cathode*

- 1 In the **Home** toolbar, click  **Functions** and choose **Global > Interpolation**.
- 2 In the **Settings** window for **Interpolation**, locate the **Definition** section.
- 3 From the **Data source** list, choose **File**.
- 4 Click  **Browse**.
- 5 Browse to the model's Application Libraries folder and double-click the file `vacancy_electromigration_cathode_concentration.txt`.
- 6 Locate the **Data Column Settings** section. In the table, click to select the cell at row number 1 and column number 1.
- 7 In the **Unit** text field, type `s`.
- 8 In the table, click to select the cell at row number 2 and column number 1.
- 9 In the **Unit** text field, type `1`.
- 10 In the **Label** text field, type `Concentration vs. Time, Cathode`.

*Concentration vs. Time, Anode*

- 1 In the **Home** toolbar, click  **Functions** and choose **Global > Interpolation**.
- 2 In the **Settings** window for **Interpolation**, locate the **Definition** section.
- 3 From the **Data source** list, choose **File**.
- 4 Click  **Browse**.

- 5 Browse to the model's Application Libraries folder and double-click the file `vacancy_electromigration_anode_concentration.txt`.
- 6 Locate the **Data Column Settings** section. In the table, click to select the cell at row number 1 and column number 1.
- 7 In the **Unit** text field, type 1.
- 8 In the table, click to select the cell at row number 2 and column number 1.
- 9 In the **Unit** text field, type 1.
- 10 In the **Label** text field, type Concentration vs. Time, Anode.

*Concentration vs. Time, Anode (int6), Concentration vs. Time, Cathode (int5), Hydrostatic Stress at t=70[s] (int1), Steady State Hydrostatic Stress (int2), Stress vs. Time, Anode (int3), Stress vs. Time, Cathode (int4)*

- 1 In the **Model Builder** window, under **Global Definitions**, Ctrl-click to select **Hydrostatic Stress at t=70[s] (int1)**, **Steady State Hydrostatic Stress (int2)**, **Stress vs. Time, Anode (int3)**, **Stress vs. Time, Cathode (int4)**, **Concentration vs. Time, Cathode (int5)**, and **Concentration vs. Time, Anode (int6)**.
- 2 Right-click and choose **Group**.


*Reference Values*

In the **Settings** window for **Group**, type Reference Values in the **Label** text field.


## GEOMETRY I

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.
- 2 In the **Settings** window for **Geometry**, locate the **Units** section.
- 3 From the **Length unit** list, choose  $\mu\text{m}$ .

*Rectangle 1 (r1)*

- 1 In the **Geometry** toolbar, click  **Rectangle**.
- 2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type Width.
- 4 In the **Height** text field, type Height.

## ADD MATERIAL

- 1 In the **Materials** toolbar, click  **Add Material** to open the **Add Material** window.
- 2 Go to the **Add Material** window.
- 3 In the tree, select **Built-in > Aluminum**.
- 4 Click the **Add to Component** button in the window toolbar.

5 In the **Materials** toolbar, click  **Add Material** to close the **Add Material** window.

Set the initial and boundary conditions for the temperature field in the Heat Transfer in Solids interface.

### HEAT TRANSFER IN SOLIDS (HT)

1 In the **Settings** window for **Heat Transfer in Solids**, locate the **Physical Model** section.

2 In the  $d_z$  text field, type Thick.

3 In the  $T_{\text{ref}}$  text field, type Tref.

#### *Initial Values 1*

1 In the **Model Builder** window, under **Component 1 (comp1) > Heat Transfer in Solids (ht)** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the  $T$  text field, type T0.

#### *Temperature 1*

1 In the **Physics** toolbar, click  **Boundaries** and choose **Temperature**.

2 Select Boundaries 1 and 4 only.

3 In the **Settings** window for **Temperature**, locate the **Temperature** section.

4 In the  $T_0$  text field, type T0.

Import additional variables to be used in the other interfaces.

### DEFINITIONS

#### *Variables 1*

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, locate the **Variables** section.

3 Click  **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `vacancy_electromigration_variables.txt`.

Set the resistivity of the interconnect and the boundary conditions for the electric field in the Electric Currents interface.

### ELECTRIC CURRENTS (EC)


1 In the **Model Builder** window, under **Component 1 (comp1)** click **Electric Currents (ec)**.

- 2 In the **Settings** window for **Electric Currents**, locate the **Thickness** section.
- 3 In the  $d$  text field, type Thick.


#### *Current Conservation I*

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Electric Currents (ec)** click **Current Conservation I**.
- 2 In the **Settings** window for **Current Conservation**, locate the **Material Type** section.
- 3 From the **Material type** list, choose **Solid**.
- 4 Locate the **Constitutive Relation Jc-E** section. From the **Conduction model** list, choose **Linearized resistivity**.
- 5 From the  $\rho_0$  list, choose **User defined**. In the associated text field, type rho\_res.
- 6 From the  $T_{ref}$  list, choose **User defined**. In the associated text field, type Tref.
- 7 From the  $\alpha$  list, choose **User defined**. In the associated text field, type alpha\_res.

#### *Ground (Anode)*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Ground**.
- 2 Select Boundary 1 only.
- 3 In the **Settings** window for **Ground**, type Ground (Anode) in the **Label** text field.

#### *Normal Current Density (Cathode)*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Normal Current Density**.
- 2 Select Boundary 4 only.
- 3 In the **Settings** window for **Normal Current Density**, locate the **Normal Current Density** section.
- 4 In the  $J_n$  text field, type -Jden.
- 5 In the **Label** text field, type Normal Current Density (Cathode).

Now you setup the transport problem adding the contribution due to Fickian's diffusion, electromigration, hydrostatic stress, and temperature.

#### **TRANSPORT IN SOLIDS (TS)**

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Transport in Solids (ts)**.
- 2 In the **Settings** window for **Transport in Solids**, locate the **Out-of-Plane Thickness** section.
- 3 In the  $d_z$  text field, type Thick.
- 4 Locate the **Transported Quantity** section. From the list, choose **Number density**.

- 5 Click to expand the **Discretization** section. From the **Transported quantity** list, choose **Linear**.


#### *Solid 1*

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Transport in Solids (ts)** click **Solid 1**.
- 2 In the **Settings** window for **Solid**, locate the **Diffusion** section.
- 3 In the  $D_c$  text field, type  $D_v$ .

#### *Initial Values 1*

- 1 In the **Model Builder** window, click **Initial Values 1**.
- 2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
- 3 In the  $c$  text field, type  $C_v0$ .


#### *Source 1*

- 1 In the **Physics** toolbar, click  **Domains** and choose **Source**.
- 2 Select Domain 1 only.
- 3 In the **Settings** window for **Source**, locate the **Sources** section.
- 4 In the  $S_c$  text field, type  $G$ .

#### *Solid 1*

In the **Model Builder** window, click **Solid 1**.

#### *Flux Due to Electric Field*

- 1 In the **Physics** toolbar, click  **Attributes** and choose **External Flux**.
- 2 In the **Settings** window for **External Flux**, locate the **External Flux** section.
- 3 Specify the  $\gamma_{\text{ext},c}$  matrix as

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PFLuxX

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PFLuxY

- 4 In the **Label** text field, type Flux Due to Electric Field.

#### *Solid 1*

In the **Model Builder** window, click **Solid 1**.

#### *Flux Due to Stress Gradient*

- 1 In the **Physics** toolbar, click  **Attributes** and choose **External Flux**.
- 2 In the **Settings** window for **External Flux**, locate the **External Flux** section.

3 Specify the  $\gamma_{\text{ext},c}$  matrix as

SFluxX

SFluxY

4 In the **Label** text field, type Flux Due to Stress Gradient.

*Solid I*

In the **Model Builder** window, click **Solid I**.

*Flux Due to Temperature Gradient*

1 In the **Physics** toolbar, click  **Attributes** and choose **External Flux**.

2 In the **Settings** window for **External Flux**, locate the **External Flux** section.

3 Specify the  $\gamma_{\text{ext},c}$  matrix as

TFluxX

TFluxY

4 In the **Label** text field, type Flux Due to Temperature Gradient.

The volumetric strain is computed from its strain rate equation using the Domain ODEs and DAEs interface.

#### **DOMAIN ODES AND DAES (DODE)**

1 In the **Model Builder** window, under **Component 1 (comp1)** click

**Domain ODEs and DAEs (dode)**.

2 In the **Settings** window for **Domain ODEs and DAEs**, click to expand the **Discretization** section.

3 From the **Shape function type** list, choose **Lagrange**.

4 Click to expand the **Dependent Variables** section. In the **Field name (1)** text field, type **ev**.

5 In the **Dependent variables (1)** table, enter the following settings:

ev

6 Locate the **Units** section. In the **Source term quantity** table, enter the following settings:

Source term quantity	Unit
Custom unit	1/s



### *Distributed ODE 1*


- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Domain ODEs and DAEs (dode)** click **Distributed ODE 1**.
- 2 In the **Settings** window for **Distributed ODE**, locate the **Source Term** section.
- 3 In the  $f$  text field, type  $\text{strate}$ .

Finally, setup the Solid Mechanics interface and add the volumetric strain from the Domain ODEs and DAEs interface.

### **SOLID MECHANICS (SOLID)**

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Solid Mechanics (solid)**.
- 2 In the **Settings** window for **Solid Mechanics**, locate the **Thickness** section.
- 3 In the  $d$  text field, type **Thick**.
- 4 Locate the **Structural Transient Behavior** section. From the list, choose **Quasistatic**.
- 5 Click to expand the **Discretization** section.


### *Fixed Constraint 1*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Fixed Constraint**.
- 2 Click in the **Graphics** window and then press Ctrl+A to select all boundaries.

### *Linear Elastic Material 1*

In the **Model Builder** window, click **Linear Elastic Material 1**.


### *External Strain 1*

- 1 In the **Physics** toolbar, click  **Attributes** and choose **External Strain**.
- 2 In the **Settings** window for **External Strain**, locate the **External Strain** section.
- 3 From the **Strain input** list, choose **Strain tensor**.
- 4 Specify the  $\epsilon_{\text{ext}}$  matrix as

$ev/3$	0	0
0	$ev/3$	0
0	0	$ev/3$

### **MESH 1**


#### *Mapped 1*

In the **Mesh** toolbar, click  **Mapped**.

### *Distribution 1*


- 1 Right-click **Mapped 1** and choose **Distribution**.
- 2 Select Boundaries 1 and 4 only.
- 3 In the **Settings** window for **Distribution**, locate the **Distribution** section.
- 4 In the **Number of elements** text field, type 30.

### *Distribution 2*

- 1 In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.
- 2 Select Boundaries 2 and 3 only.
- 3 In the **Settings** window for **Distribution**, locate the **Distribution** section.
- 4 From the **Distribution type** list, choose **Predefined**.
- 5 In the **Number of elements** text field, type 50.
- 6 In the **Element ratio** text field, type 4.
- 7 Select the **Symmetric distribution** checkbox.
- 8 Click  **Build All**.


## **STUDY 1**

### *Step 1: Time Dependent*


- 1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.
- 2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.
- 3 In the **Output times** text field, type 0 40 50 60 70 80 range(500,500,3500) 24000 25200 26000 range(40000,10000,190000) range(200000,100000,1400000).
- 4 In the **Study** toolbar, click  **Compute**.

## **RESULTS**

### *Surface 1*



- 1 In the **Model Builder** window, expand the **Transported Quantity (ts)** node, then click **Surface 1**.
- 2 In the **Settings** window for **Surface**, locate the **Expression** section.
- 3 In the **Expression** text field, type  $c/Cv0$ .
- 4 In the **Transported Quantity (ts)** toolbar, click  **Plot**.

### *Cut Line 2D 1*

- 1 In the **Results** toolbar, click  **Cut Line 2D**.

- 2 In the **Settings** window for **Cut Line 2D**, locate the **Line Data** section.
- 3 In row **Point 1**, set **y** to 7.5.
- 4 In row **Point 2**, set **x** to 100.
- 5 In row **Point 2**, set **y** to 7.5.

#### *Hydrostatic Stress (Centerline) at 70 s*

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Cut Line 2D 1**.
- 4 From the **Time selection** list, choose **From list**.
- 5 In the **Times (s)** list box, select **70**.
- 6 In the **ID Plot Group 7** toolbar, click  **Plot**.
- 7 In the **Label** text field, type Hydrostatic Stress (Centerline) at 70 s.
- 8 Click to expand the **Title** section. From the **Title type** list, choose **Label**.
- 9 Locate the **Plot Settings** section.
- 10 Select the **y-axis label** checkbox. In the associated text field, type Hydrostatic stress (N/cm<sup>2</sup>).

#### *Model Results*

- 1 Right-click **Hydrostatic Stress (Centerline) at 70 s** and choose **Line Graph**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type -solid.pm.
- 4 In the **Unit** field, type N/cm<sup>2</sup>.
- 5 Click to expand the **Legends** section. Select the **Show legends** checkbox.
- 6 From the **Legends** list, choose **Manual**.
- 7 In the table, enter the following settings:

---

#### **Legends**

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Model Results

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- 8 In the **Label** text field, type Model Results.

#### *Results for Validation*

- 1 In the **Model Builder** window, right-click **Hydrostatic Stress (Centerline) at 70 s** and choose **Line Graph**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

- 3 In the **Expression** text field, type  $\text{int1}(x)$ .
- 4 In the **Unit** field, type  $\text{N}/\text{cm}^2$ .
- 5 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
- 6 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.
- 7 From the **Positioning** list, choose **Interpolated**.
- 8 Locate the **Legends** section. Select the **Show legends** checkbox.
- 9 From the **Legends** list, choose **Manual**.
- 10 In the table, enter the following settings:


---

#### **Legends**

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#### Reference


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- 11 In the **Label** text field, type Results for Validation.
- 12 In the **Hydrostatic Stress (Centerline) at 70 s** toolbar, click  **Plot**.


#### *Hydrostatic Stress at Steady State (Centerline)*

- 1 Right-click **Hydrostatic Stress (Centerline) at 70 s** and choose **Duplicate**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Data** section.
- 3 From the **Time selection** list, choose **Last**.
- 4 In the **Label** text field, type Hydrostatic Stress at Steady State (Centerline).

#### *Results for Validation*

- 1 In the **Model Builder** window, expand the **Hydrostatic Stress at Steady State (Centerline)** node, then click **Results for Validation**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type  $\text{int2}(x)$ .
- 4 In the **Hydrostatic Stress at Steady State (Centerline)** toolbar, click  **Plot**.


#### *Cut Point 2D, Anode*

- 1 In the **Results** toolbar, click  **Cut Point 2D**.
- 2 In the **Settings** window for **Cut Point 2D**, locate the **Point Data** section.
- 3 In the **x** text field, type 0.
- 4 In the **y** text field, type 7.5.
- 5 In the **Label** text field, type Cut Point 2D, Anode.

### *Cut Point 2D, Cathode*

- 1 Right-click **Cut Point 2D, Anode** and choose **Duplicate**.
- 2 In the **Settings** window for **Cut Point 2D**, locate the **Point Data** section.
- 3 In the **x** text field, type 50.
- 4 In the **Label** text field, type Cut Point 2D, Cathode.

### *Hydrostatic Stress vs. Time*

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Hydrostatic Stress vs. Time in the **Label** text field.
- 3 Locate the **Title** section. From the **Title type** list, choose **Label**.
- 4 Locate the **Plot Settings** section.
- 5 Select the **y-axis label** checkbox. In the associated text field, type Hydrostatic stress (N/cm<sup>2</sup>).
- 6 Locate the **Legend** section. From the **Position** list, choose **Middle right**.

### *Model Results Anode*

- 1 Right-click **Hydrostatic Stress vs. Time** and choose **Point Graph**.
- 2 In the **Settings** window for **Point Graph**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Cut Point 2D, Anode**.
- 4 Locate the **y-Axis Data** section. In the **Expression** text field, type -solid.pm.
- 5 In the **Unit** field, type N/cm<sup>2</sup>.
- 6 Locate the **x-Axis Data** section. From the **Unit** list, choose **d**.
- 7 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.
- 8 In the table, enter the following settings:

---

**Legends**

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Model Results, Anode

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- 9 Select the **Show legends** checkbox.
- 10 In the **Label** text field, type Model Results Anode.

### *Model Results Cathode*

- 1 Right-click **Model Results Anode** and choose **Duplicate**.
- 2 In the **Settings** window for **Point Graph**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Cut Point 2D, Cathode**.

4 Locate the **Legends** section. In the table, enter the following settings:

---

**Legends**

---

Model Results, Cathode

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5 In the **Label** text field, type Model Results Cathode.

*Reference*

1 In the **Model Builder** window, right-click **Hydrostatic Stress vs. Time** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **x-Axis Data** section.

3 From the **Unit** list, choose **d**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:


Expression	Unit	Description
int3(t)	N/cm <sup>2</sup>	Reference, Anode
int4(t)	N/cm <sup>2</sup>	Reference, Cathode

5 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

6 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

7 From the **Positioning** list, choose **Interpolated**.

8 In the **Label** text field, type Reference.

9 In the **Hydrostatic Stress vs. Time** toolbar, click  **Plot**.

*Normalized Concentrations vs. Time*

1 Right-click **Hydrostatic Stress vs. Time** and choose **Duplicate**.

2 In the **Settings** window for **ID Plot Group**, type Normalized Concentrations vs. Time in the **Label** text field.

3 Locate the **Plot Settings** section. In the **y-axis label** text field, type Normalized concentration (1).

*Model Results Anode*

1 In the **Model Builder** window, expand the **Normalized Concentrations vs. Time** node, then click **Model Results Anode**.

2 In the **Settings** window for **Point Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type  $ts.c/Cv0$ .

*Model Results Cathode*

1 In the **Model Builder** window, click **Model Results Cathode**.

- 2 In the **Settings** window for **Point Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type `ts.c/Cv0`.

*Reference*

- 1 In the **Model Builder** window, click **Reference**.
- 2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
<code>int6(t)</code>		Reference, Anode
<code>int5(t)</code>	1	Reference, Cathode

- 4 In the **Normalized Concentrations vs. Time** toolbar, click  **Plot**.

